Spectrum Generation in NISTMonte

Accurate x-ray spectrum simulation depends upon reliable models of the many different physical processes involved in electron-generated x-ray emission. A lack of understanding of any of the following: electron scattering, x-ray absorption, inner-shell ionization, x-ray emission, or Bremsstrahlung emission will lead to simulated spectra that differ from measured spectra. These differences can be used as clues to identify flaws in and to refine the underlying models. NIST has developed a Monte Carlo simulation of electron transport to facilitate trying and assessing new models. Most microanalytical measurements made today rely on the understanding of these underlying models.

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It has long been understood that the best way to quantify x-ray spectra is by comparison with reference standard spectra. However, collecting standards is time consuming. In reality, most spectra measured in industrial labs are quantified using quicker and less accurate standardless methods. Standardless methods work reasonably when the measured x-ray transitions are from the same family (K, L, or M shell). However because of limitations in our understanding of inner-shell ionization cross sections, the method is not reliable when the transitions are from different families. While the best measurements are likely always to be based on comparison with standards, there is a real need to improve the quality of standardless analysis.

NISTMonte, a Monte Carlo simulation of electron transport recently developed at NIST, has been enhanced to include spectrum simulation capabilities based on the best available models. NISTMonte has been designed as a framework that facilitates trying new or alternative models. Characteristic x-ray generation is modeled via one of a handful of different expressions for ionization cross section, fluorescence yield, and relative line intensity. Bremsstrahlung is modeled using tabulated cross sections from Seltzer and Berger. (Seltzer S, Berger M, Atom. Data and Nucl Data Tables, **35**, 1986 pp 345-418). The spectra are output in a format compatible with most x-ray and microanalysis quantification software.

NISTMonte provides a framework for developing new models to improve the accuracy of microanalytical measurements used in a wide range of industries and applications from R&D to quality control.

NISTMonte has been enhanced to generate simulated x-ray spectra based on the best available physical models. Fig. 1 shows the excellent agreement between a simulated x-ray spectrum from NISTMonte for NIST analytical glass K3189 and an experimentally measured spectrum.

Microanalytical measurements are important in research and development, manufacturing, and quality control in a wide range of industries. In-as-much as these techniques give incorrect answers, there remains the potential for economically inefficient decisions. Since standardless analysis is widely used by industry; there is a basic economic argument for improving the accuracy in these techniques.

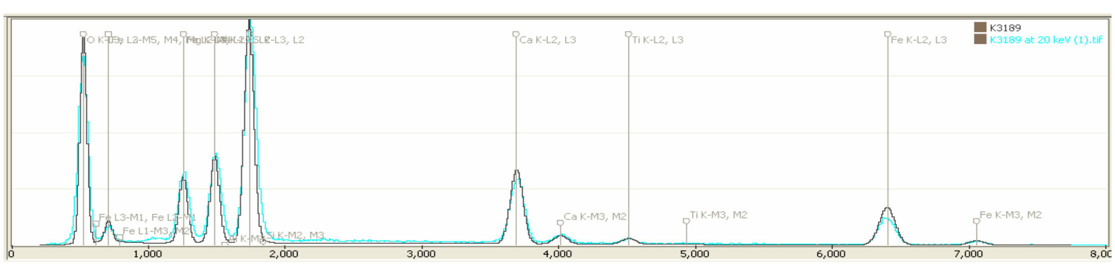

Fig. 1: Comparing a simulated and measured spectrum from K3189 glass measured at 20 keV

Future plans: Spectra generated using NISTMonte will be compared with measured spectra. Models will be refined as a result of these comparisons. These models will be back-propagated into improved standardless quantification algorithms.